Spectral gap of the totally asymmetric exclusion process at arbitrary filling

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Abstract

We calculate the spectral gap of the Markov matrix of the totally asymmetric simple exclusion process (TASEP) on a ring of L sites with N particles. Our derivation is simple and self-contained and extends a previous calculation that was valid only for half-filling. We use a special property of the Bethe equations for TASEP to reformulate them as a one-body problem. Our method is closely related to the one used to derive exact large deviation functions of the TASEP.

Keywords: ASEP, Bethe Ansatz, Dynamical Exponent, Spectral Gap.

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1 Introduction

The asymmetric simple exclusion process (ASEP) is a driven diffusive system of particles on a lattice interacting through hard-core exclusion, that serves as a basic model in various fields ranging from protein synthesis to traffic flow

(for a recent review, see Schütz 2001). In non-equilibrium statistical physics, the ASEP plays the role of a paradigm thanks to the variety of phenomenological behavior it displays and to the number of exact results it has led to in the last decade (see, *e.g.*, Derrida 1998). In particular, ASEP is an integrable model, *i.e.*, the Markov matrix that encodes its stochastic dynamics can be diagonalized by Bethe Ansatz, as first noticed by Dhar (1987). Thus, the spectral gap of the Markov matrix, *i.e.*, the difference between the two eigenvalues with largest real parts, that characterizes the longest relaxation time of the system, can be calculated exactly: this was first done for the totally asymmetric simple exclusion process (TASEP) at half filling (Gwa and Spohn 1992) and later, using a mapping into the six vertex model, Kim (1995) treated the case of the general ASEP at arbitrary filling. In both works, the calculations are complicated though the final result for the gap is fairly simple. In a recent work (Golinelli and Mallick 2004), we presented a concise derivation of the TASEP gap at half filling that circumvents most of the technical difficulties thanks to an analytic continuation formula. However, the half filling condition seemed to play a crucial role in our derivation (as well as in the calculation of Gwa and Spohn). Our aim in the present work is to show that our method can be extended to the arbitrary filling case.

We shall study the TASEP on a periodic one-dimensional lattice with L sites (sites i and $L+i$ are identical). The TASEP is a discrete lattice gas model on which each lattice site i ($1 \le i \le L$) is either empty or occupied by one particle (*exclusion rule*). Particles evolve according to stochastic dynamical rules: a particle on a site i at time t jumps, in the interval between times t and $t+dt$, with probability dt to the neighbouring site $i+1$ if this site is empty. As the system is periodic, the total number N of particles is conserved and the density (or filling) is given by $\rho = N/L$. A configuration of the TASEP can be characterized by the positions of the N particles on the ring, $(x_1, x_2, \ldots, x_N)$ with $1 \le x_1 < x_2 < \ldots < x_N \le L$. If $\psi_t(x_1, \ldots, x_N)$ represents the probability of this configuration at time t, the evolution of ψ_t is given by the master equation $d\psi_t/dt = M\psi_t$, where M is the Markov matrix. A right eigenvector ψ is associated with the eigenvalue E of M if $M\psi = E\psi$. Thanks to the Perron-Frobenius theorem, we know that the zero-eigenvalue of M, which corresponds to the stationary state, is non-degenerate and that all the other eigenvalues of M have a strictly negative real part. In the stationary state, all configurations have the same probability, given by $N!(L-N)!/L!$.

In the next section, we present the Bethe Ansatz equations and restate them as a single self-consistency equation. We then calculate the TASEP spectral gap as a function of the density ρ in the limit of a large system size, $L \to \infty$ (Section 3).

2 The Bethe Ansatz Equations

The *Bethe Ansatz* assumes that the eigenvectors ψ of M can be written in the form

$$\psi(x_1, \ldots, x_N) = \sum_{\sigma \in \Sigma_N} \mathcal{A}_\sigma \, z_{\sigma(1)}^{x_1} \, z_{\sigma(2)}^{x_2} \ldots z_{\sigma(N)}^{x_N} \,, \tag{1}$$

where Σ_N is the group of the $N!$ permutations of N indexes. The coefficients $\{\mathcal{A}_\sigma\}$ and the wave-numbers $\{z_1, \ldots, z_N\}$ are complex numbers determined by the *Bethe equations*. In terms of the fugacity variables $Z_i = 2/z_i - 1$, these equations become (Gwa and Spohn 1992)

$$(1 - Z_i)^N \, (1 + Z_i)^{L-N} = -2^L \prod_{j=1}^{N} \frac{Z_j - 1}{Z_j + 1} \quad \text{with} \quad i = 1, \ldots, N \,. \tag{2}$$

We note that the right-hand side of these equations is independent of the index i: this property is true only for the *totally* asymmetric exclusion process and not for the partially asymmetric exclusion process where the particles can also jump backwards. Introducing an auxiliary complex variable Y, the Bethe equations (2) can be reformulated as explained below (for more details, see Gwa and Spohn 1992; Golinelli and Mallick 2004). Consider the one variable polynomial equation of degree L,

$$(1 - Z)^N \, (1 + Z)^{L-N} = Y \,, \tag{3}$$

and call $(Z_1, Z_2, \ldots, Z_L)$ the L roots of this equation. For a given value of Y, the complex numbers $(Z_1, Z_2, \ldots, Z_L)$ belong to a generalized Cassini oval defined by the equation

$$|Z - 1|^\rho \, |Z + 1|^{1-\rho} = r \quad \text{with} \quad r = |Y|^{1/L} \,, \tag{4}$$

ρ being the density of the system. The topology of the Cassini oval depends on the value of r (see the figure). Defining

$$r_c = 2\rho^\rho (1 - \rho)^{(1-\rho)} \,, \tag{5}$$

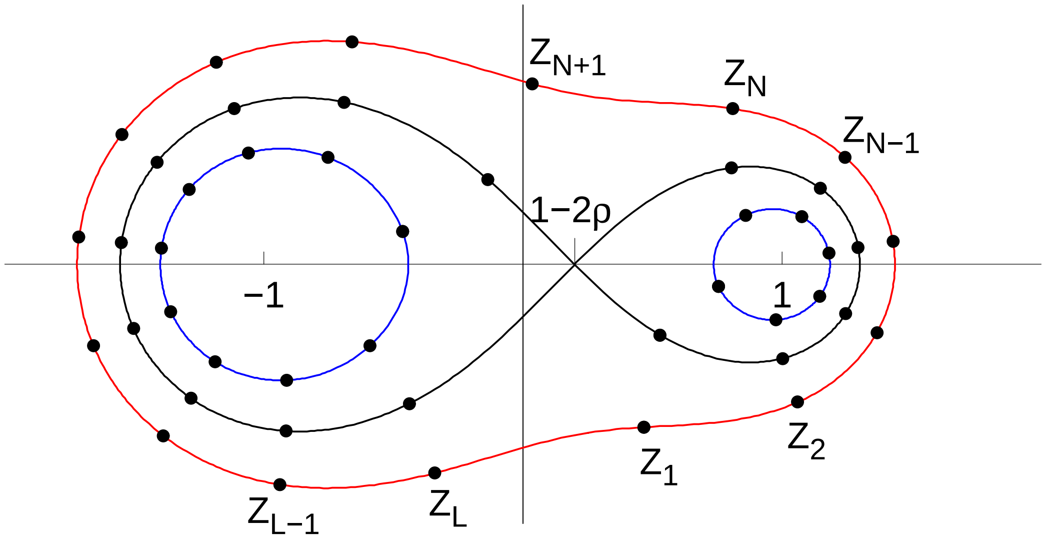

Figure 1: *Roots of the equation* $(1-Z)^N(1+Z)^{L-N} = Y$*. Here* $N = 6$ *and* $L = 15$ *(the filling is* $\rho = 2/5$*) with* $Y = e^{i\phi}r^L$ *for* $\phi = \pi/2$*; curves are drawn for* $r/r_c = 0.8$ *(blue),* 1 *(black) and* 1.2 *(red). See text for more explanations.*

we find that for $r < r_c$, the locus of the Z's consists of two disjoint ovals, with the roots $(Z_1, Z_2, \ldots, Z_N)$ belonging to the oval on the right and the roots $(Z_{N+1}, Z_{N+2}, \ldots, Z_L)$ to the oval on the left. For $r = r_c$, the Cassini oval is a deformed lemniscate of Bernoulli with a double point at $Z_c = 1-2\rho$. For $r > r_c$, the oval is made of a single loop. The labelling of the L roots $(Z_1, \ldots, Z_L)$ is shown in the figure.

We now introduce a monotonous function $c : \{1, \ldots, N\} \to \{1, \ldots, L\}$ that selects N fugacities among the L roots $(Z_1, \ldots, Z_L)$. Defining the function $A_c(Y)$ as

$$A_c(Y) = -2^L \prod_{j=1}^{N} \frac{Z_{c(j)} - 1}{Z_{c(j)} + 1}\,, \qquad (6)$$

the Bethe equations become equivalent to the *self-consistency* equation

$$A_c(Y) = Y\,. \qquad (7)$$

Given the choice function c and a solution Y of this equation, the $Z_{c(j)}$'s are determined from Eq. (3) and the corresponding eigenvalue E_c is given by

$$2E_c = -N + \sum_{j=1}^{N} Z_{c(j)}\,. \qquad (8)$$

The choice function $c_0(j) = j$ that selects the N fugacities Z_i with the largest real parts provides the ground state of the Markov matrix. The associated A-function and eigenvalue are given by

$$A_0(Y) = -2^L \prod_{j=1}^{N} \frac{Z_j - 1}{Z_j + 1}, \tag{9}$$

$$2E_0 = -N + \sum_{j=1}^{N} Z_j \,. \tag{10}$$

The equation $A_0(Y) = Y$ has the unique solution $Y = 0$ that yields $Z_j = 1$ for $j \leq N$ and provides the ground state with eigenvalue 0. We shall also need the following formula in the sequel:

$$\ln \frac{A_0(Y)}{Y} = -\frac{L}{N} \sum_{j=1}^{N} \ln\left(\frac{1 + Z_j}{2}\right) . \tag{11}$$

To derive this identity, we raise equation (9) to the N-th power, use equation (3) and take the logarithm of the result; however an additional term, which is a discrete constant (a multiple of $2i\pi/N$) appears in the calculations. This constant vanishes identically because both terms in equation (11) become real numbers in the limit $Y \to 0$.

The spectral gap, given by the first excited eigenvalue, corresponds to the choice $c_1(j) = j$ for $j = 1, \ldots, N-1$ and $c_1(N) = N + 1$ (Gwa and Spohn 1992). The associated self-consistency function and eigenvalue are given by (using equations (6, 8-10))

$$A_1(Y) = A_0(Y) \frac{Z_{N+1} - 1}{Z_{N+1} + 1} \, \frac{Z_N + 1}{Z_N - 1}, \tag{12}$$

$$2E_1 = 2E_0 + (Z_{N+1} - Z_N) \,. \tag{13}$$

Thus, from equation (12), the self-consistency equation that determines the gap reads

$$0 = \ln \frac{A_1(Y)}{Y} = \ln \frac{A_0(Y)}{Y} - \ln\left(\frac{1 - Z_N}{1 + Z_N} \, \frac{1 + Z_{N+1}}{1 - Z_{N+1}}\right) . \tag{14}$$

The excitation corresponding to the choice function $c(j) = j + 1$ for $j = 1, \ldots, N-1$ and $c(N) = L$, leads to the complex-conjugate eigenvalue $\bar{E}_1$. The eigenvalue E_1 corresponding to the first excited state is obtained by solving the self-consistency equation $A_1(Y) = Y$ where A_1 is defined in equation (12). We shall solve this equation in the limit $N, L \to \infty$, keeping $\rho = N/L$ constant.

3 Calculation of the first excited state

As in (Golinelli and Mallick 2004), we start with the Taylor expansions, of $A_0(Y)$ and $E_0(Y)$ in the vicinity of $Y = 0$ and valid for arbitrary values of N and L. In our previous work, we considered only the half-filling case, $L = 2N$, for which the polynomial equation (3) reduces to $(1 - Z^2)^N = Y$ and can be solved *explicitly* in terms of Y yielding the Taylor series of A_0 and E_0. An explicit solution of equation (3) can not, however, be obtained for an arbitrary density ρ. This major technical difficulty can be circumvented thanks to a contour integral representation similar to that used for calculating large deviation functions (Derrida and Lebowitz 1998; Derrida and Appert 1999; Derrida and Evans 1999).

When $Y \to 0$, the N roots $(Z_1, \ldots, Z_N)$ of equation (3) with the largest real parts converge to +1, whereas the $L - N$ remaining roots converge to -1. We now consider a positively oriented contour γ that encircles +1 such that for sufficiently small values of Y the roots $(Z_1, \ldots, Z_N)$ lie inside γ and $(Z_{N+1}, \ldots, Z_L)$ are outside γ. Let $h(Z)$ be a function that is analytic in a domain containing the contour γ. We also define

$$P(Z) = (1 - Z)^N \ (1 + Z)^{L-N}. \tag{15}$$

Because, by definition, the Z_j are the zeroes of $P(Z) = Y$, we obtain, from the residues theorem,

$$\sum_{m=1}^{N} h(Z_m) = \frac{1}{2i\pi} \oint_\gamma \frac{P'(Z)}{P(Z) - Y} h(Z) \mathrm{d}Z \,. \tag{16}$$

Expanding the denominator in the contour integral for small values of Y (thanks to the formula $(P - Y)^{-1} = \sum_{k=0}^{\infty} Y^k / P^{k+1}$ valid for $|Y| < |P|$), we obtain the Taylor expansion

$$\begin{aligned}
\sum_{m=1}^{N} h(Z_m) &= \frac{1}{2i\pi} \sum_{k=0}^{\infty} Y^k \oint_\gamma \frac{P'(Z)}{P^{k+1}(Z)} h(Z) \, \mathrm{d}Z \\
&= \frac{1}{2i\pi} \oint_\gamma \frac{P'(Z)}{P(Z)} h(Z) \, \mathrm{d}Z + \frac{1}{2i\pi} \sum_{k=1}^{\infty} \frac{Y^k}{k} \oint_\gamma \frac{h'(Z)}{P^k(Z)} \mathrm{d}Z \\
&= N h(1) + \frac{1}{2i\pi} \sum_{k=1}^{\infty} \frac{Y^k}{k} \oint_\gamma \frac{h'(Z) \, \mathrm{d}Z}{(1 - Z)^{kN} (1 + Z)^{k(L-N)}} \,.
\end{aligned} \tag{17}$$

The second equality is derived by integrating by parts the terms with $k \geq 1$; the term $Nh(1)$ in the third equality is obtained from the residues theorem. We shall need the following identity, valid for any positive integers P and Q:

$$\frac{1}{2i\pi} \oint_\gamma \frac{1}{(1-Z)^P (1+Z)^Q} \, \mathrm{d}Z = -2^{1-P-Q} \left(\begin{array}{c} P+Q-2 \\ P-1 \end{array} \right) . \tag{18}$$

Using equation (17) with $h(Z) = \ln\left(\frac{1+Z}{2}\right)$, we obtain from equations (11) and (18)

$$\ln \frac{A_0(Y)}{Y} = \sum_{k=1}^{\infty} \left(\begin{array}{c} kL \\ kN \end{array} \right) \frac{Y^k}{k 2^{kL}} . \tag{19}$$

Similarly, using equation (17) with $h(Z) = Z - 1$, we obtain from equations (10) and (18)

$$2E_0 = -\sum_{k=1}^{\infty} \left(\begin{array}{c} kL-2 \\ kN-1 \end{array} \right) \frac{Y^k}{k 2^{kL-1}} . \tag{20}$$

In the limit $L \to \infty$ and with ρ fixed, we obtain from the Stirling formula

$$\ln \frac{A_0(Y)}{Y} \to \frac{1}{\sqrt{2\pi\rho(1-\rho)L}} \, \mathrm{Li}_{3/2}\left(\frac{Y}{r_c^L} \right) , \tag{21}$$

where r_c was defined in equation (5) and the *polylogarithm* function of index s, Li_s, is given by

$$\mathrm{Li}_s(z) = \frac{z}{\Gamma(s)} \int_0^\infty \frac{t^{s-1} \, dt}{e^t - z} = \sum_{k=1}^{\infty} \frac{z^k}{k^s} . \tag{22}$$

The function Li_s is defined by the first equality on the whole complex plane with a branch cut along the real semi-axis $[1, +\infty)$; the second equality is valid only for $|z| < 1$.

The limit found in equation (21) suggests that Y can be parameterized as follows:

$$Y = -r_c^L e^{u\pi} , \tag{23}$$

u being a complex number with $-1 \leq \mathrm{Im}(u) < 1$ and which remains finite in the limit $L \to \infty$. Thus $|Y|^{1/L} \simeq r_c$ and roots of the type Z_k, Z_{L-k} and $Z_{N\pm k}$ where k is a fixed positive integer are close to the lemniscate double-point

$Z_c = 1 - 2\rho$. Writing $Z = 1 - 2\rho + 2\xi$, with $\xi \ll 1$, and taking the logarithm of equation (2) we obtain

$$(1-\rho)\ln\left(1+\frac{\xi}{1-\rho}\right) + \rho\ln\left(1-\frac{\xi}{\rho}\right) = \pi\frac{u+i(2k-1)}{L}\,. \tag{24}$$

For fixed k, the values $k \leq 0$ lead to Z_{N-k} and Z_{L-k}, and $k \geq 1$ lead to Z_k and Z_{N+k}. Neglecting terms of order $\mathcal{O}\left(L^{-3/2}\right)$, we have

$$Z_N = 1 - 2\rho + 2i\sqrt{\frac{2\pi\rho(1-\rho)}{L}}\,(u-i)^{1/2} + \frac{4\pi}{3}\frac{1-2\rho}{L}(u-i) + \ldots \tag{25}$$

$$Z_{N+1} = 1 - 2\rho + 2i\sqrt{\frac{2\pi\rho(1-\rho)}{L}}\,(u+i)^{1/2} + \frac{4\pi}{3}\frac{1-2\rho}{L}(u+i) + \ldots \tag{26}$$

Substituting equations (21), (25) and (26) in equation (14), we obtain the large L limit of the Bethe equations for the gap which, at the leading order, reads as

$$\mathrm{Li}_{3/2}(-e^{u\pi}) = 2i\pi\left[(u+i)^{1/2} - (u-i)^{1/2}\right]. \tag{27}$$

This equation is the same as that obtained in (Golinelli and Mallick 2004) and its solution is given by:

$$u = 1.119\,068\,802\,804\,474\ldots \tag{28}$$

We can now calculate the eigenvalue corresponding to the first excited state. ¿From equations (13), (14) and (20), we obtain

$$2E_1 = (2E_0 + Z_{N+1} - Z_N) + 2\rho(1-\rho)\ln\frac{A_1(Y)}{Y} = \tag{29}$$

$$-\sum_{k=1}^{\infty}\frac{\rho(1-\rho)\begin{pmatrix} kL \\ kN \end{pmatrix}Y^k}{k(kL-1)2^{kL-1}} + (Z_{N+1} - Z_N) - 2\rho(1-\rho)\ln\frac{(1-Z_N)(1+Z_{N+1})}{(1+Z_N)(1-Z_{N+1})}\,.$$

The large L limit of this expression is found by using the Stirling formula, the expansions (25) and (26), and the parameterization of Y given by equation (23). We thus obtain

$$\begin{aligned} 2E_1 = \quad & -\frac{1}{L^{3/2}}\sqrt{\frac{2\rho(1-\rho)}{\pi}}\left(\mathrm{Li}_{5/2}(-e^{u\pi}) - \frac{4\pi^2}{3}i\left[(u+i)^{3/2} - (u-i)^{3/2}\right]\right) \\ & + \frac{4i\pi}{L}(1-2\rho)\,, \end{aligned} \tag{30}$$

where u is the solution of the equation (27), its numerical value being given in equation (28). Comparing with the value $E_{1,\,\rho=1/2}$ obtained at half-filling we conclude that

$$E_1 = 2\sqrt{\rho(1-\rho)}\; E_{1,\,\rho=1/2} + \frac{2i\pi}{L}(1-2\rho)\,. \tag{31}$$

This equation agrees with the one derived by Kim (1995). We notice that this eigenvalue has a non-vanishing imaginary part when the density is different from one half.

4 Conclusion

The asymmetric exclusion process can be mapped into the six vertex model and is thus an integrable model that can be solved by Bethe Ansatz. Kim (1995) has used this technique to calculate gaps and crossover functions for the generic asymmetric exclusion process but the calculations are very complicated. However, for the totally asymmetric exclusion process the Bethe equations can be reduced to a single polynomial equation and their analysis becomes much simpler as shown in the present work. We have calculated the gap of the TASEP for arbitrary filling. Our method is closely related to that used to calculate large deviation functions (see Derrida 1998, for a review) and leads to derivations that are far simpler than the ones presented in previous works. This technique can be generalized to calculate any finite excitation close to the ground state of the system.

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